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## References

- [1] Takeshi Nishimatsu, Umesh V. Waghmare, Yoshiyuki Kawazoe, and David Vanderbilt. Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective hamiltonian. *Phys. Rev. B*, 78:104104, Sep 2008.
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- [3] Takeshi Nishimatsu, Masaya Iwamoto, Yoshiyuki Kawazoe, and Umesh V. Waghmare. First-principles accurate total energy surfaces for polar structural distortions of \${\text{BaTiO}}\_{3}\$, \${\text{PbTiO}}\_{3}\$, and \${\text{SrTiO}}\_{3}\$: Consequences for structural transition temperatures. 82(13):134106.
- [4] Takeshi Nishimatsu, Masaya Iwamoto, Yoshiyuki Kawazoe, and Umesh V. Waghmare. First-principles accurate total energy surfaces for polar structural distortions of BaTiO<sub>3</sub>, PbTiO<sub>3</sub>, and SrTiO<sub>3</sub>: Consequences for structural transition temperatures. 82(13):134106.